

Directed branched polymers near an attractive line

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2004 J. Phys. A: Math. Gen. 37 3673

(<http://iopscience.iop.org/0305-4470/37/11/009>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.90

The article was downloaded on 02/06/2010 at 17:50

Please note that [terms and conditions apply](#).

Directed branched polymers near an attractive line

Sumedha

Department of Theoretical Physics, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai 400 005, India

E-mail: sumedha@theory.tifr.res.in

Received 4 November 2003, in final form 29 January 2004

Published 2 March 2004

Online at stacks.iop.org/JPhysA/37/3673 (DOI: 10.1088/0305-4470/37/11/009)

Abstract

We study the adsorption–desorption phase transition of a directed branched polymer in $d + 1$ dimensions in contact with a line by mapping it to a d -dimensional hard core lattice gas at negative activity. We solve the model exactly in $1 + 1$ dimensions, and calculate the crossover exponent related to the fraction of monomers adsorbed at the critical point of the surface transition, and we also determine the density profile of the polymer in different phases. We also obtain the value of the crossover exponent in $2 + 1$ dimensions and give the scaling function of the sticking fraction for $(1 + 1)$ - and $(2 + 1)$ -dimensional directed branched polymer.

PACS numbers: 05.50.+q, 05.40.Fb, 82.35.–x

Linear and branched polymers, near an attractive surface, undergo an adsorption–desorption transition, which has important applications in areas ranging from technology such as that in lubrication, adhesion and surface protection to biology [1, 2]. For example, adsorbed polymers are used for surface modification of medical implants [3]. There have been several theoretical studies of the behaviour of a polymer near a surface [2, 4–8]. In particular, the effect of a surface for an idealized polymer (with no self-exclusion), modelled by random walks, has been studied extensively. There are many exact results known for Gaussian random walks in the presence of a surface [9, 10]. In comparison, linear polymers with self-exclusion and branched polymers are less well studied. For a self-avoiding walk (SAW) in the vicinity of a surface, the exact critical exponents are known from conformal field theory [11]. Directed polymer chain adsorption, modelled by a directed SAW, is one of the few solvable models of surface effects in two and three dimensions [6]. For directed walks, self-exclusion is automatic, and nontrivial effects of excluded volume interaction are not seen. For branched polymers (modelled by lattice animals), a relation between the exponent characterizing the number of animals in the presence of a surface and in the bulk is known from a simple argument given by De’Bell *et al* [12]. In this paper we solve for a directed branched polymer (DBP) in two dimensions and three dimensions in the presence of a 1D (one-dimensional) line, exactly. Introducing

a preferred direction makes the system analytically more tractable. Similar results for two dimensions have also been obtained by Rensburg and Rechnitzer [13] independently.

The enumeration of directed site animals in $d + 1$ dimensions is related to hard core lattice gas (HCLG) at negative activity with repulsive interactions in d dimensions and the Yang–Lee edge problem in d dimensions [14–17]. In this paper we give the mapping of a $(d + 1)$ -dimensional DBP in the presence of a line to a d -dimensional HCLG with repulsive interactions.

The plan of the paper is as follows. In section 1 we will define the model of a DBP and the quantities of interest. Using the above mentioned correspondence we give the mapping of a $(d + 1)$ -dimensional DBP in the presence of a line to a d -dimensional HCLG with repulsive interactions in section 2. In section 3, for a $(1 + 1)$ -dimensional DBP in the presence of a 1D penetrable line we solve the model exactly. Section 4 deals with the DBP in $1 + 1$ dimensions in the presence of an impenetrable line. For a DBP in $1 + 1$ dimensions we show that the behaviours at the transition point for penetrable and impenetrable walls are the same—not just the crossover exponents: even the density profiles are the same. This implies that for $1 + 1$ dimensions, for an impenetrable surface, at the phase transition point the decrease in entropy is exactly compensated by the increase in internal energy. This seems to be a special property of polymers in two dimensions. Even for linear polymers, the exponents for the two cases are the same and hence it is believed that for a linear polymer in two dimensions in the presence of an impenetrable surface the phase transition point corresponds to a point where surface effects vanish completely and the system behaves like a bulk [8]. Here we are able to show this explicitly for a DBP. In section 5, using Baxter’s solution for a hard hexagon gas, we study a $(2 + 1)$ -dimensional DBP in the presence of a line and calculate the crossover exponent and sticking fraction for the DBP exactly. The scaling function of the sticking fraction is a function of two intensive thermodynamic variables. We have derived its exact form in $1 + 1$ dimensions and $2 + 1$ dimensions. There are very few such exact nontrivial scaling functions of more than one thermodynamic variable known [18]. We also get the large w expansion of the sticking fraction as a power series in $1/\sqrt{w}$.

1. The model

A DBP or a directed animal on a lattice, rooted at the origin, is a connected cluster such that any site of the animal can be reached from the root by a walk which never proceeds oppositely to the preferred direction. For example, on a square lattice drawn tilted at 45° in figure 1, a directed site animal or a DBP \mathcal{A} rooted at the origin is a set of occupied sites including the origin such that for each occupied site (x, t) other than the origin, at least one of the two sites $(x - 1, t - 1)$ and $(x + 1, t - 1)$ is also occupied. The number of sites in \mathcal{A} will be denoted by $s = |\mathcal{A}|$. We define $n(x|\mathcal{A})$ as the number of sites of \mathcal{A} having the transverse coordinate x . We study the DBP in the presence of a 1D line parallel to the preferred direction. This is positioned along the main diagonal of the lattice (figure 1). We will consider only polymers rooted at the surface in this paper.

We assign a fugacity y to all allowed sites of the cluster. Further, if we associate an additional energy $-E$ with each site on the surface, each site on surface will have an additional weight and the fugacity of sites about the diagonal, denoted by y_0 , is equal to wy where

$$w = \exp(E/kT). \quad (1)$$

Hence $w > 1$ would correspond to an attractive surface.

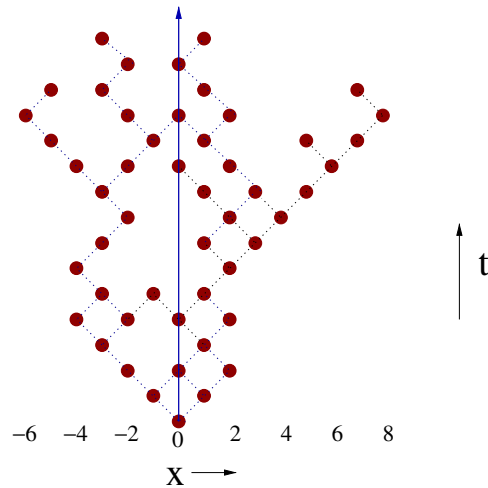


Figure 1. A DBP of size 50, rooted on the surface.

We define $A(w, y)$, the grand partition function of the polymer, as

$$A(w, y) = \sum_{\mathcal{A}} y^{|\mathcal{A}|} w^{n_0} = \sum_{s=1}^{\infty} A_s(w) y^s \tag{2}$$

where $n_0 = n(0|\mathcal{A})$ and $A_s(w)$ is the partition function of the polymer made up of exactly s monomers.

For $w = 1$, we get the statistics of equally weighted animals and $A_s(1)$ is the number of distinct directed animals having s sites with given boundary conditions. For large s , $A_s(w)$ varies as $\lambda^s s^\theta$, where θ is known as the entropic critical exponent. Similarly, the transverse size of the polymer for large s scales as s^ν , where ν is the exponent which defines the transverse length scale of the polymer. These exponents take different values in desorbed, adsorbed and critical regions. We will use subscripts de, c and ad to represent critical exponents and other quantities in desorbed, critical and adsorbed phases of the polymer.

And the free energy per monomer of the polymer in thermodynamic limit is given by

$$F(T) = \lim_{s \rightarrow \infty} - \frac{k_B T}{s} \log A_s(w) \equiv k_B T \log(y_\infty(w)) \tag{3}$$

where $y_\infty(w)$ is the value of the fugacity at which $A(w, y)$ has a singularity for a given value of w .

Let $\phi(\mathbf{x}, s)$ be the value of $n(\mathbf{x}, \mathcal{A})$ averaged over all configurations \mathcal{A} of size s . We define a generating function $\Psi(\mathbf{x}; w, y)$ as

$$\Psi(\mathbf{x}; w, y) = \sum_{\mathcal{A}} n(\mathbf{x}|\mathcal{A}) w^{n_0} y^{|\mathcal{A}|} \equiv \sum_s \phi(\mathbf{x}, s) A_s(w) y^s. \tag{4}$$

There is a critical value w_c of wall activity such that for $w > w_c$, $\phi(0, s)$ is proportional to s for large s and the transverse size is finite ($\nu_{ad} = 0$). This is the adsorbed phase, in which monomers tend to stick to the surface. $w < w_c$ corresponds to the desorbed phase of the polymer in which only a finite number of monomers stick to the surface. At $w = w_c$, the critical point of the surface transition, the number of adsorbed monomers as a function of the polymer size in the large s limit has a behaviour given by

$$\phi_c(0, s) \sim s^\alpha \tag{5}$$

where α is known as the crossover exponent of the surface transition.

In the $s \rightarrow \infty$ limit, the fraction of monomers adsorbed is like an order parameter of the surface phase transition. In the constant fugacity ensemble, $A(w, y)$ is the partition function with fixed w and y and hence the average polymer size would be given by

$$\langle s(y, w) \rangle = \frac{\sum s y^s w^{n_0}}{\sum y^s w^{n_0}} \equiv \frac{\partial \ln A(w, y)}{\partial \ln y}. \quad (6)$$

Similarly, the average number of monomers at the surface would be

$$\langle n_0(y, w) \rangle = \frac{\sum n_0 y^s w^{n_0}}{\sum y^s w^{n_0}} \equiv \frac{\partial \ln A(w, y)}{\partial \ln w}. \quad (7)$$

The sticking fraction defined as the fraction of polymer segments at the surface, represented by $C_{st}(w, y)$, would be given by

$$C_{st}(w, y) = \frac{\langle n_0(y, w) \rangle}{\langle s(y, w) \rangle}. \quad (8)$$

In the infinite polymer limit, if we represent the value of the fugacity at which $\langle s(y, w) \rangle$ diverges by $y_\infty(w)$ for a given w , then the sticking fraction is only a function of the wall activity w and is given by

$$C_{st}(w) = -\frac{d \ln y_\infty(w)}{d \ln w}. \quad (9)$$

This is the order parameter of the surface phase transition and is zero for $w \leq w_c$, where w_c is the surface phase transition point.

In general, in the large polymer limit, near the critical value of w , as $w \rightarrow w_c^+$, $C_{st}(w, y)$ is expected to have the scaling form

$$C_{st}(w, y) = \epsilon^{1-\alpha} h((w - w_c)\epsilon^{-\alpha}) \quad (10)$$

where $\epsilon = 1 - y/y_\infty(w)$. The scaling function $h(u)$, where $u = (w - w_c)\epsilon^{-\alpha}$, is a function of w and y which are both intensive thermodynamic variables. As $u \rightarrow \infty$, $h(u) \sim u^{(1-\alpha)/\alpha}$.

2. General results

The directed site animal enumeration (DSAE) problem in $d + 1$ dimensions is related to the time development of the thermal relaxation of a HCLG with nearest neighbour exclusion on a d -dimensional lattice [15]. In [19], we have shown that this correspondence relates the density at a site i in the steady state to the sum of weights of all animals rooted at i , the grand partition function of the animal. Also, the average number of sites at a given transverse distance \mathbf{x} from the origin for a $(d + 1)$ -dimensional directed animal is related to the density–density correlation function of the lattice gas in d dimensions.

Specifically, if on a $(d + 1)$ -dimensional body-centred hypercubic lattice we define the weight of an animal \mathcal{A} as the product of the weights of all occupied sites, with the weight corresponding to a site with \mathbf{x} coordinate i being y_i , then the DSAE problem on this $(d + 1)$ -dimensional lattice becomes related to the time development of the HCLG with nearest neighbour exclusion on a d -dimensional body-centred hypercubic lattice with rates which satisfy the detailed balance condition corresponding to the Hamiltonian

$$H = +\infty \sum_{\langle ij \rangle} n_i n_j - \sum_i (\ln z_i) n_i \quad (11)$$

where $z_i = -y_i/(1 + y_i)$ and the animal number generating function is just the negative of the density of the HCLG with the change of variables from z to y . Here we have used the convention that if $\sum_{\langle ij \rangle} n_i n_j = 0$, then the corresponding term in the Hamiltonian is zero.

The configurations with any pair of occupied nearest neighbours have infinite energy and do not contribute to the partition function.

The partition function is linear in all z_i . The linearity of the partition function in the z_i implies that in the case where the activity about $\mathbf{x} = 0$ is different from that in the rest of the sample, i.e. if we let the activity about $\mathbf{x} = 0$ be z_0 and the activity in the rest of the space be z , then the partition function of the HCLG can be written as

$$Z(z_0, z) = A(z) + z_0 B(z) \tag{12}$$

where $A(z)$ and $B(z)$ are polynomials in z . If ρ represents the density of the HCLG when the activities about each of the sites are the same, then the density of the HCLG about the origin in the present case $\rho_0(z_0, z)$ can be written in terms of ρ as

$$\rho_0(z_0, z) = \frac{z_0 \rho}{\rho z_0 + z(1 - \rho)}. \tag{13}$$

The same observation has been made by Cardy in [20]. Correspondingly, since $A(w, y)$ is just the negative of $\rho_0(z_0, z)$ with $z_0 = -wy/(1 + wy)$ and $z = -y/(1 + y)$, we can express $A(w, y)$ in terms of $A(1, y)$ and this is given by

$$A(w, y) = \frac{w(1 + y)A(1, y)}{(1 + wy) + A(1, y)(1 - w)}. \tag{14}$$

Moreover, the density–density correlation function of the HCLG $G(\mathbf{x}; w, z)$ with $w \neq 1$ can be expressed in terms of the density–density correlation function when $w = 1$. We find that the density–density correlation function is related to $\Psi(\mathbf{x}; w, y)$ on a hypercubic lattice as follows:

$$\Psi(\mathbf{x}; w, y) = -\frac{1}{1 + y} G\left(\mathbf{x}; w, z = \frac{-y}{1 + y}\right). \tag{15}$$

From this we get

$$\frac{\Psi(\mathbf{x}; w, y)}{\Psi(\mathbf{x}; 1, y)} = \frac{w(1 + y)[1 + wy - (1 - A(1, y))(1 - w)]}{[1 + wy + A(1, y)(1 - w)]^2}. \tag{16}$$

Since ρ is the density of the HCLG, then, as discussed in [19], for $\mathbf{x} = 0$, the density–density correlation of the HCLG is always equal to $\rho(\rho - 1)$ for any d -dimensional case and hence $\Psi(0; 1, y)$ can be completely expressed in terms of $A(1, y)$. Hence we get

$$\Psi(0; w, y) = \frac{w(1 + y)A(1, y)(1 + A(1, y))}{[1 + wy + A(1, y)(1 - w)]^2}. \tag{17}$$

Equations (14)–(17) hold for all dimensions. Hence, in the presence of a 1D surface, a DBP in $d + 1$ dimensions rooted on the surface can be studied using the mapping to the HCLG. Moreover, the generating functions $A(w, y)$ and $\Psi(0; w, y)$ can be completely expressed in terms of the animal number generating function when the wall is neutral, i.e., in terms of $A(1, y)$. We will use these results in the rest of the paper to study the surface effects for a DBP in two and three dimensions.

In the adsorbed regime the number of monomers in direct contact with the wall is proportional to s and $\nu_{\text{ad}} = 0$. This implies that the scaling form of $\phi(\mathbf{x}, s)$ in the adsorbed regime is

$$\phi_{\text{ad}}(\mathbf{x}, s) \sim \frac{s}{\xi^d} g(|\mathbf{x}|/\xi) \tag{18}$$

where $\xi = (w - w_c)^{\bar{\nu}}$ is the characteristic length scale in the system. Since we are away from the critical regime, ξ is well behaved and never diverges for finite w . Also ξ is independent of the size s of the polymers. The normalization of the scaling function $g(r)$ is chosen such that

$$\int_{-\infty}^{\infty} d^d \mathbf{x} g(|\mathbf{x}|) = 1. \tag{19}$$

$A_s(w)\phi(\mathbf{x}, s)$ is the coefficient of y^s in the expansion of $\Psi(\mathbf{x}; w, y)$. In the adsorbed regime, $A_s(w) \sim (y_\infty(w))^{-s}$ for large s and the behaviour of $\phi(\mathbf{x}, s)$ is given by equation (18); hence $\Psi(\mathbf{x}; w, y)$ will have a scaling form

$$\Psi(\mathbf{x}; w, y) \sim \frac{\epsilon^{-2}}{\xi^d} g(|\mathbf{x}|/\xi) \quad (20)$$

where $\epsilon = 1 - y/y_\infty(w)$.

Since the scaling function $g(|\mathbf{x}|/\xi)$ has no y dependence, the scaling function of $G(\mathbf{x}; w, z)$ would also be just $g(|\mathbf{x}|/\xi)$ for $w > w_c$.

3. The two-dimensional DBP in the presence of a 1D penetrable surface

For a penetrable surface, since configurations spanning through the surface are allowed, there is no loss of entropy per monomer to take into account (figure 1). Hence, $w = 1$ corresponds to a zero gain in free energy per monomer of the surface. We find a value of y at which $A(1, y)$ diverges; the only value of w which makes $A(w, y)$ also divergent is $w = 1$. This implies that $w_c = 1$ for a DBP in any dimension in the presence of a 1D line as long as $A(1, y)$ becomes singular at a finite value of y . Then the polymer has bulk behaviour at the critical point. At $w = 1$, i.e. for a DBP in the bulk, we have shown in an earlier paper [19] by scaling arguments and dimensional analysis that $\phi(\mathbf{x}, s)$ has a scaling form

$$\phi_c(\mathbf{x}, s) \sim s^{1-d\nu_c} f(|\mathbf{x}|\epsilon^{-\nu_c}). \quad (21)$$

This implies that $\phi_c(0, s) \sim s^{1-d\nu_c}$, and the crossover exponent α is exactly given by

$$\alpha = 1 - d\nu_c \equiv 1 - \theta \quad (22)$$

where ν_c is the transverse correlation exponent of a $(d + 1)$ -dimensional directed animal in the bulk, which is equal to the correlation length exponent for a d -dimensional HCLG with nearest neighbour exclusion.

As we go to higher dimensions, even though entropy loss and energy gain balance each other at $w = 1$, the polymer might start binding to a line only for wall activity greater than 1. For DBP, when $A(1, y)$ has no divergence, $w = 1$ is not the critical point of the surface transition. Instead it is given by

$$w_c = \frac{1 + 1/A(1, y_c)}{1 - y_c/A(1, y_c)} \quad (23)$$

where y_c is the large polymer limit fugacity value of the polymer with a neutral wall, i.e., when $w = 1$.

As an example, on a Bethe lattice with coordination number 3, the function $A(1, y)$ is

$$A_B(1, y) = \frac{1 - \sqrt{1 - 4y}}{2y} \quad (24)$$

and $y_c = 1/4$. At $y = 1/4$ the function $A_B(1, y) = 2$, and substituting in equation (23) we get $w_c = 12/7$, which is greater than 1.

The $(1 + 1)$ -dimensional directed animal gets mapped to a 1D HCLG. For $(1 + 1)$ -dimensional directed animals in the bulk, in [19] we have derived the exact expressions for $A(1, y)$ and $\Psi(x; 1, y)$. Using them and equations (14)–(16) we get the expressions for $A(w, y)$ and $\Psi(x; w, y)$ as follows:

$$A(w, y) = \frac{2wy(1 + y)}{(1 - y - wy - 3wy^2) + (1 + wy)\sqrt{(1 - 3y)(1 + y)}}. \quad (25)$$

The connected density–density correlation function of the corresponding gas is a simple exponential and hence the generating function $\Psi(x; w, y)$ has the form

$$\Psi(x; w, y) = K(w, y) \exp(-b(y)|x|) \quad (26)$$

where it is straightforward to calculate $K(w, y)$ and $b(y)$, and we get

$$K(w, y) = \frac{2wy(1-3y)(1+wy)(1-y+\sqrt{(1-3y)(1+y)})}{[(1-3y)(1+wy)\sqrt{1+y} + (1-y-wy-3wy^2)\sqrt{1-3y}]^2} \quad (27)$$

and

$$b(y) = \log(\sqrt{1+y} + \sqrt{1-3y}) - \log(\sqrt{1+y} - \sqrt{1-3y}). \quad (28)$$

The generating functions $A(w, y)$ and $\Psi(x; w, y)$ have branch cuts at $y = 1/3$. For $w = 1$, they also have a pole singularity at $y = 1/3$. Hence, clearly the phase transition from the desorbed to the adsorbed phase occurs at $w = 1$, i.e. $w_c = 1$. For $w \leq 1$, $y_\infty(w) = 1/3$, while for $w > 1$, it is given by the real positive solution of

$$w - y - w(3+2w)y^2 - 3w^2y^3 = 0. \quad (29)$$

Near the critical point, for $w = 1 + \delta$, to leading order we get $y_\infty(w)$ as

$$y_\infty(w) = \frac{1}{3} - \frac{\delta^2}{16} + \text{higher order terms}. \quad (30)$$

The sticking fraction $C_{\text{st}}(w, y)$ can also be exactly calculated and we get it as

$$C_{\text{st}}(w, y) = \left[\frac{y(1-w)}{1+y} + \frac{1+wy}{\sqrt{(1+y)(1-3y)}} \right]^{-1}. \quad (31)$$

From this, near the critical point, we get the scaling form of $C_{\text{st}}(w, y)$ as

$$C_{\text{st}}(w, y) = \sqrt{\epsilon} h(u) \quad (32)$$

where $\epsilon = 1 - y/y_\infty(w)$ and $u = \epsilon^{-1/2}\delta$ and we get

$$h(u) = \frac{\sqrt{3}}{2} \left[1 + \frac{9u^2}{48} \right]^{\frac{1}{2}}. \quad (33)$$

This gives the order parameter $C_{\text{st}}(w)$ near the critical point as proportional to $\frac{3\delta}{8}$. For large values of w , expanding $C_{\text{st}}(w)$ in powers of $(1/w)$ we get

$$C_{\text{st}}(w) \sim \frac{1}{2} - \frac{3\sqrt{2}}{16\sqrt{w}} - \frac{3}{16w} - \dots \quad (34)$$

For $w \rightarrow \infty$ this approaches $1/2$, the maximum possible fraction that can stick to wall, as expected.

4. The two-dimensional DBP in the presence of a 1D impenetrable surface

In the presence of an impenetrable surface, because of the loss in entropy for each monomer on the wall, the transition from the desorbed to the adsorbed phase takes place at a nontrivial value of the adsorption activity.

Here we study a DBP in $1+1$ dimensions on a square lattice, in the presence of an impenetrable surface, about the diagonal (figure 2). From the exact generating functions $A(1, y)$, $A(w, y)$ and $\Psi(x; w, y)$, it is straightforward to determine the critical value of w , the sticking fraction and the density profile in the desorbed, critical and adsorbed phases of the system. The $(1+1)$ -dimensional case in the presence of a solid wall along the growth direction

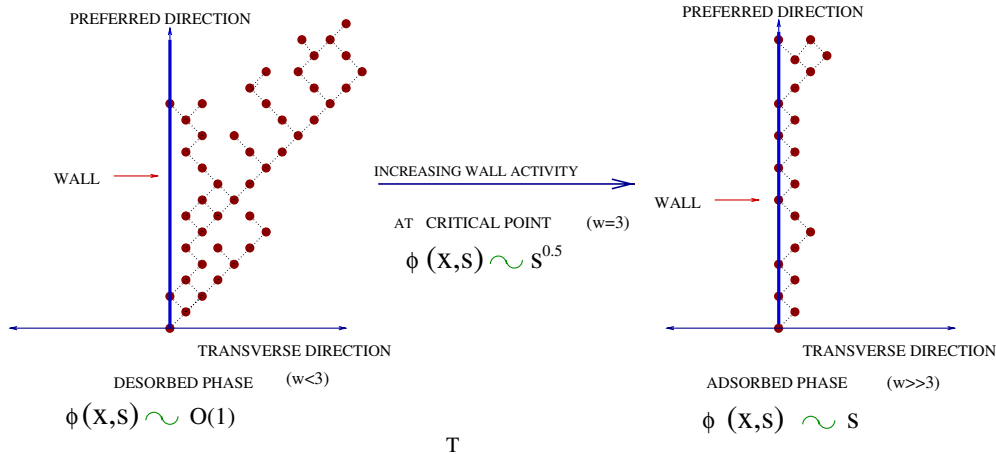


Figure 2. A DBP on a square lattice in the presence of a 1D impenetrable line, about the diagonal.

can be mapped to the HCLG in 1D with fugacity 0 for all sites lying along the negative axis. Making use of this mapping we get

$$A(1, y) = \frac{(1 - y - \sqrt{1 - 2y - 3y^2})}{2y} \tag{35}$$

and $A(w, y)$ is easy to get by substituting in equation (14). This result can also be obtained using the heap method. For an alternative treatment, see [13].

The density–density correlation of the corresponding gas is exponential and hence the generating function $\Psi(x; w, y)$ still has the form given by equation (26), but $K(w, y)$ and $b(y)$ are now given by

$$K(w, y) = \frac{wy(1 + wy)(\sqrt{1 + y} + \sqrt{1 - 3y})}{(1 + y)(1 - w^2y^2)\sqrt{1 - 3y} + (1 - y - (4 - w)wy^2 - w^2y^3)\sqrt{1 + y}} \tag{36}$$

and

$$b(y) = \log(\sqrt{1 + y} + \sqrt{1 - 3y}) - \log(\sqrt{1 + y} - \sqrt{1 - 3y}). \tag{37}$$

The generating functions $A(w, y)$ and $\Psi(x; w, y)$ have a branch cut at $y = 1/3$. At $w = 1$, $A(1, y)$ has no divergence and $y_c = 1/3$. Substituting in equation (23), we get $w_c = 3$. This value is greater than the value for a (1 + 1)-dimensional DBP with a penetrable surface. This is expected, since the tendency of a polymer to grow away from the surface is more pronounced when the surface is impenetrable and hence only when the surface becomes sufficiently attractive does the polymer start sticking to it. For $w > 3$, the closest singularity to the origin occurs at

$$y_s = \frac{\sqrt{4w - 3} - 1}{2w}. \tag{38}$$

For $w \leq 3$ the branch cut singularity $1/3$ dominates and hence $y_\infty(w)$, the infinite polymer limit fugacity value, is equal to $1/3$ for $w \leq 3$, whereas for $w > 3$, $y_\infty(w) = y_s$. The free energy is a constant and the order parameter, $C_{st}(w)$, is zero for $w < 3$.

We get the sticking fraction, $C_{st}(w, y)$, as

$$C_{st}(w, y) = \frac{1 - 2y - 3y^2 + (-1 + y + 2y^2)\sqrt{(1 + y)(1 - 3y)}}{y[-2y + (w + 2y - wy)\sqrt{(1 + y)(1 - 3y)} + w(-1 + 2y + 2y^2)]}. \tag{39}$$

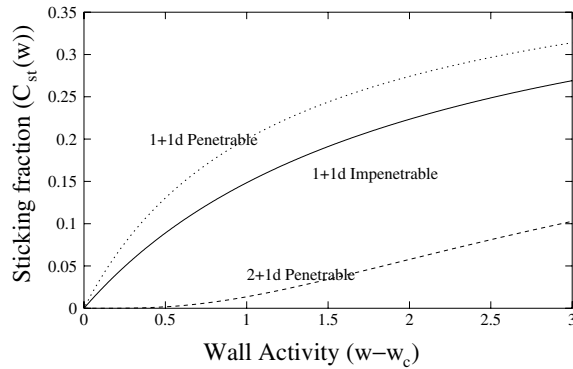


Figure 3. The sticking fraction in the presence of a line for a DBP in 1 + 1 and 2 + 1 dimensions, when the polymer size tends to infinity.

Near the critical point for $w = 3 + \delta$ and $y = y_s(1 - \epsilon)$, we get the same scaling form for $C_{st}(w, y)$ as given by equation (32), with the scaling function $h(u)$ as

$$h(u) = \frac{2}{\sqrt{3}} \left[1 + \frac{u^2}{27} \right]^{\frac{1}{2}}. \tag{40}$$

Hence $C_{st}(w)$ is proportional to $\frac{2\delta}{9}$ near the critical point and approaches 1/2 as $w \rightarrow \infty$. This is plotted in figure 3 along with the sticking fraction for the penetrable case. The qualitative behaviours in the two cases are almost the same, the main difference being the shift of the transition point from 1 to 3 and the initial slope. For large values of w it is easy to expand $C_{st}(w)$ in powers of $1/w$. It should be noted that the large w expansion of $C_{st}(w)$ will involve powers of $w^{-1/2}$ in this case as well.

Using the exact equations for the generating function for $\Psi(x; w, y)$ we translate these results to the constant number ensemble and we get the function $\phi(x, s)$ in three regions giving the spread of sites as a function of distance from the wall. Here we give these calculations for the impenetrable case only, because the qualitative behaviours in the impenetrable and penetrable cases are exactly same for a (1 + 1)-dimensional system.

In the desorbed phase ($w < 3$), expanding near $y_c = 1/3$ as $y = y_c e^{-\epsilon}$, we get the scaling form for $\Psi(x; w, y)$ as

$$\Psi(x; w, \epsilon) = c(w) \exp(-x\sqrt{3\epsilon}), \tag{41}$$

where $c(w)$ is a w dependent constant and is $\frac{3(3+w)}{2(3-w)^2}$.

To obtain $\phi(x, s)$ for large s , we need to determine the coefficient of y^s in the series expansion of $\Psi(x; w, \epsilon)$, i.e.,

$$\Psi(x; w, \epsilon) \equiv \sum_s \phi(\mathbf{x}, s) A_s(w) y^s = c(w) \sum_{k=0}^{\infty} \frac{(-\sqrt{3}x)^k}{\Gamma[k+1]} (1-3y)^{\frac{k}{2}} \tag{42}$$

$$= c(w) \sum_{s=0}^{\infty} (3y)^s \sum_{k=0}^{\infty} \frac{(-\sqrt{3}x)^k}{\Gamma[k+1]} \frac{\Gamma[s-k/2]}{\Gamma[s+1]\Gamma[-k/2]}. \tag{43}$$

For fixed k and large s ,

$$\frac{\Gamma[s-k/2]}{\Gamma[s+1]} \rightarrow s^{-1-k/2}. \tag{44}$$

Hence the leading singular behaviour of $\phi(x, s)A_s(w)$ in the desorbed phase is given by

$$\phi(x, s)A_s = \frac{3^s c(w)}{s} \sum_{k=0}^{\infty} \frac{(-\sqrt{3}x/\sqrt{s})^k}{\Gamma[k+1]\Gamma[-k/2]}. \quad (45)$$

Since $\Gamma[-k/2]$ has poles when k is an even integer, only odd terms contribute to the sum. It is easy to sum the resulting series, giving $\phi(x, s)$ for large s in the desorbed phase as

$$\phi_{\text{de}}(x, s) = \frac{3}{2}x \exp\left(-\frac{3x^2}{4s}\right). \quad (46)$$

For $w = 3$, $c(w)$ is singular and we have to keep terms up to first order in ϵ in the expansion (for $w < 3$ the constant term dominates) and we get

$$\Psi(x; 3, \epsilon) = \frac{1}{\epsilon} \exp(-x\sqrt{3\epsilon}). \quad (47)$$

Again, just as in the desorbed phase, expanding $\Psi(x; 3, \epsilon)$ in powers of y^s , the average number of sites at a distance x , i.e. $\phi(x, s)$ for the critical region for large s , is found to be

$$\phi(x, s) = \frac{\sqrt{3\pi s}}{2} \operatorname{erfc}\left(\frac{\sqrt{3}x}{2\sqrt{s}}\right). \quad (48)$$

Hence we see that at $w = 3$ it is not just that the crossover exponent α is equal to $1/2$; even the scaling form of $\phi(x, s)$ is the same as that of a $(1+1)$ -dimensional directed animal in bulk [19] and hence the same as that of the penetrable wall at the critical point. This unusual result can be understood as coming from the exact cancellation of the decrease in entropy and increase in internal energy at the critical point. Also, note that the value of the exponent $\alpha = 1/2$ for DBP is equal to the estimates of α for branched polymers [21] and linear polymers [22] in two dimensions. In fact, for adsorption of an undirected d -dimensional branched polymer on a $(d-1)$ -dimensional surface, the crossover exponent α is conjectured to be $1/2$ in all spatial dimensions [23].

For $w > 3$, the behaviour of the generating function is dominated by the singularity given by equation (38). For $w \gg 3$, $y_s \approx 1/\sqrt{w}$ and we get the large s behaviour of $\phi(x, s)$ as

$$\phi(x, s) = s \exp(-x) \quad (49)$$

i.e., most of the sites stick to the origin as expected.

Similarly, expanding $A(w, y)$ about y_c and then going to a constant number (s) ensemble, we get $A_s(w)$ for large s as $A_s(w) \sim \frac{\sqrt{3}}{2\sqrt{\pi}}c(w)3^s s^{-\frac{3}{2}}$ in the desorbed regime. Hence the numbers of animals in the presence of the 1D impenetrable wall, i.e. $A_s(1)$ for large s , are $A_s(1) \sim \frac{\sqrt{3}}{2\sqrt{\pi}}3^s s^{-\frac{3}{2}}$. This gives θ_{de} as $3/2$. This is consistent with the result derived for lattice trees by De'Bell *et al* [12]. Also we get at the critical point $w = 3$, $A_s(3) \sim \frac{2}{\sqrt{3\pi}}3^s s^{-\frac{1}{2}}$, implying θ_c to be $1/2$. For $w \gg 3$, $A_s(w) \sim (\sqrt{w})^s$, giving $\theta_{\text{ad}} = 0$.

The function $\phi(x, s)$ gives the density profile of the polymer as a function of distance from the surface. Since the configurations are very different in the two phases as shown schematically in figure 2, the $\phi(x, s)$ are very different in the three regions. In the desorbed phase $\phi(x, s)$ peaks away from the surface at a distance of the order of the average transverse diameter of the polymer in the large s limit, whereas at the critical point it peaks at the surface (figure 4).

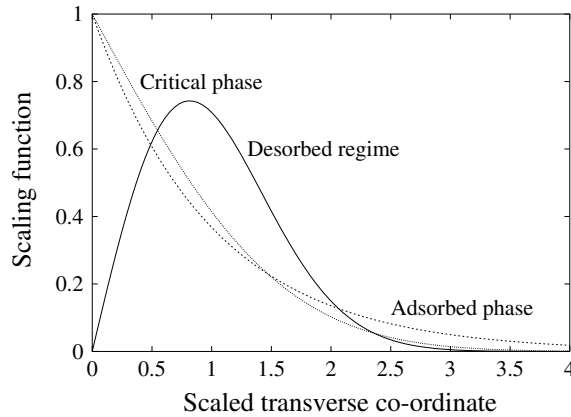


Figure 4. The density profile of a two-dimensional DBP in the presence of a 1D surface.

5. A three-dimensional DBP in the presence of an attractive line

In 2 + 1 dimensions, a DBP on a simple cubic lattice with nearest and next nearest neighbour connections gets mapped to the hard hexagon gas model in two dimensions at negative activity in the disordered regime; this problem was solved by Baxter [24]. He obtained the equation for the average density of the gas. It was shown by Joyce that there is an algebraic equation in z (the activity of the gas) and ρ (the density of the gas) [25].

The equation given by Joyce is quartic in z and twelfth order in ρ . For convenience we will just reproduce it here [25]:

$$\rho(1 - \rho)^{11} - (1 - \rho)^5 P_1(\rho)z + \rho^2(1 - \rho)^2 P_2(\rho)z^2 - \rho^5 P_1(\rho)z^3 + \rho^{11}(1 - \rho)z^4 = 0 \quad (50)$$

where

$$P_1(\rho) = (1 - 13\rho + 66\rho^2 - 165\rho^3 + 220\rho^4 - 165\rho^5 + 77\rho^6 - 22\rho^7)$$

$$P_2(\rho) = (1 - 13\rho + 63\rho^2 - 125\rho^3 + 6\rho^4 + 401\rho^5 - 689\rho^6 + 476\rho^7 - 119\rho^8).$$

The density ρ of the HCLG is just the negative of $A(1, y)$ and $z = -y/(1 + y)$. It is straightforward to get an algebraic equation in $A(1, y)$ as a function of y [26]. As $A(w, y)$ is a simple rational function of $A(1, y)$, y and w (see equation (14)), replacing ρ in $A(w, y)$, the grand partition function of the (2 + 1)-dimensional directed animal in the presence of a one-dimensional line about the main diagonal of the lattice, we get a twelfth-order polynomial equation in $A(w, y)$, where the coefficients are functions of w and y . Explicitly writing down the equation is rather tedious and this is omitted. Since $A(1, y)$ becomes singular for $y = y_c = 2/(9 + 5\sqrt{5})$, in the presence of a 1D line the polymer will undergo a desorption-adsorption transition at $w = 1$. For $w \leq 1$ the dominant singularity will be y_c and $y_\infty(w) = y_c$. For $w > 1$, at $y_\infty(w)$, $A(w, y)$ tends to infinity and at this point the coefficient of the highest order term must be zero. Since we have a twelfth-order equation in $A(w, y)$, by equating the coefficient of the twelfth-order term to zero, we get a polynomial equation in y and w ($Q(y, w) = 0$) whose smallest positive real root is $y_\infty(w)$. This polynomial is twelfth order in w . But we can find the root numerically. The free energy is just $\log(y_\infty(w))$ and hence can be evaluated numerically.

In this case the expressions for $A(w, y)$ and other generating functions are rather complicated and hence it is difficult to go to the constant size ensemble. But at the critical point the system behaves like the bulk and, since $\theta = 5/6$, by hyperscaling arguments, $\nu_c = 5/12$,

which implies that the crossover exponent $\alpha = 1/6$ (equation (22)). And by equation (10), the sticking fraction $C_{st}(w, y) \sim (1 - y/y_\infty(w))^{5/6}$ as $w \rightarrow 1^+$ asymptotically.

By solving $Q(y, w) = 0$ we get $y_\infty(w)$ as a function of w . Near the critical point for $w = 1 + \delta$, to leading order we get

$$y_\infty(w) = y_c(1 - c\delta^6 + \text{higher order term}) \quad (51)$$

where $c = 5(5\gamma)^5$ with $\gamma = (13\sqrt{5} - 25)/50$.

In the large polymer limit, for y very close to y_c , $A(1, y)$ has a scaling form

$$A(1, y) = a_0 \left(1 - \frac{y}{y_c}\right)^{-\frac{1}{6}} \left[1 + a_1 \left(1 - \frac{y}{y_c}\right)^{\frac{5}{6}} + \dots\right] \quad (52)$$

where $a_0 = (\sqrt{5}\gamma^{1/6})^{-1}$ [26].

Hence taking $y = y_\infty(w)(1 - \epsilon)$ and $w = 1 + \delta$ we get the scaling function of $C_{st}(w, y) = \epsilon^{5/6}h(u)$ as

$$h(u) = \frac{6a_0}{1 + y_c} (1 + cu^6)^{\frac{5}{6}} - 6cu^5 \quad (53)$$

where $u = \delta\epsilon^{-1/6}$. The scaling function $h(u)$ is a function of w and y , which are both thermodynamic variables.

For large w , expanding in powers of $1/w$ we get

$$y_\infty(w) \sim \frac{1}{\sqrt{6w}} - \frac{1}{4w} - \frac{11}{16}\sqrt{\frac{3}{2}}\left(\frac{1}{w}\right)^{\frac{3}{2}} - \dots \quad (54)$$

and

$$C_{st}(w) \sim \frac{1}{2} - \frac{1}{4}\sqrt{\frac{3}{2w}} - \frac{9}{4w} - \dots \quad (55)$$

As $w \rightarrow \infty$, $C_{st}(w)$ approaches $1/2$, the maximum possible fraction of adsorption. It is like an order parameter of the surface transition. It is plotted in figure 3. As is clear from the scaling function, the sticking fraction increases much more slowly than in the $(1+1)$ -dimensional case. This is expected, as there the polymer in $d+1$ dimensions was being adsorbed on a d -dimensional surface, whereas here a polymer in $d+1$ dimensions is being adsorbed on a $(d-1)$ -dimensional surface.

Acknowledgments

I am very grateful to my advisor Professor Deepak Dhar for guidance at every step of this work. I acknowledge the partial financial support received from the TIFR Alumni Association Scholarship.

References

- [1] Eisenriegler E 1993 *Polymer Near Surfaces* (Singapore: World Scientific)
- [2] Vanderzande C 1998 *Lattice Models of Polymers (Cambridge Lecture Notes in Physics)* (Cambridge: Cambridge University Press)
- [3] Norde I 1995 *Surface and Interfacial Aspects of Biomedical Applications* (New York: Plenum)
- [4] De'Bell K and Lookman T 1993 *Rev. Mod. Phys.* **65** 87
- [5] Stella A L and Vanderzande C 1990 *Int. J. Mod. Phys. B* **4** 1437
- [6] Privman V, Forgacs G and Frisch H L 1988 *Phys. Rev. B* **37** 9897
- [7] Mishra P K, Kumar S and Singh Y 2003 *Physica A* **323** 453

- [8] Bouchaud E and Vannimenus J 1989 *J. Physique* **50** 2931
- [9] Rubin R J 1965 *J. Chem. Phys.* **43** 2392
- [10] Majumdar S N 1990 *Physica A* **169** 207
- [11] Duplantier B and Saleur H 1986 *Phys. Rev. Lett.* **57** 3179
- [12] De'Bell K, Lookman T and Zhao D 1991 *Phys. Rev. A* **44** 1390
- [13] Rensburg E J and Rechnitzer 2001 *J. Stat. Phys.* **105** 49
- [14] Cardy J L 1982 *J. Phys. A: Math. Gen.* **15** L593
- [15] Dhar D 1983 *Phys. Rev. Lett.* **51** 853
- [16] Lai S and Fisher M E 1995 *J. Chem. Phys.* **103** 8144
Park Y and Fisher M E 1999 *Phys. Rev. E* **60** 6323
- [17] Brydges D C and Imbrie J Z 2001 *Preprint math-ph/0107005*
- [18] Cardy J 2001 *J. Phys. A: Math. Gen.* **34** L665
- [19] Sumedha and Dhar D 2003 *J. Phys. A: Math. Gen.* **36** 3701
- [20] Cardy J 2003 *Preprint cond-mat/0302495*
- [21] de Queiroz S L A 1995 *J. Phys. A: Math. Gen.* **28** 6315
You S and Rensburg E J 2001 *Phys. Rev. E* **64** 046101
- [22] Guim I and Burkhardt T W 1988 *J. Phys. A: Math. Gen.* **22** 1131
- [23] Janssen H K and Lyssy A 1994 *Phys. Rev. E* **50** 3784
- [24] Baxter R J 1979 *J. Phys. A: Math. Gen.* **13** L61
- [25] Joyce G S 1988 *J. Phys. A: Math. Gen.* **21** L983
- [26] Joyce G S 1989 *J. Phys. A: Math. Gen.* **22** L919